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TABLE OF CONTENTS

	Page
I. Objective	2
II. Background and Approach	2
III. [REDACTED] Research	4
A. Energy Growth and Ionization in Driven Atomic Systems	4
a) The Time-Periodic Case	4
b) General Time Dependence	5
c) Dissociation by Chirped Laser Pulses	5
B. Transport Processes in Plasmas	6
1. Bounds on the Mobility of Electrons in Weakly Ionized Plasmas	6
2. The Reflection of Electromagnetic Waves by a Conducting Surface Shielded with a Plasma Layer	7
C. Phase Transitions and Instabilities	9
1. Phase Transitions in a Spatially Uniform Weakly Ionized Plasma	9
2. Phase Transition in a Cylindrical Plasma	11
3. Transitions between Shear and Vortex Flows in Statistical Hydrodynamics	13
4. Instabilities in Plasmas Interacting with Lasers	14
D. Phase Segregation Dynamics in Particle Systems with Long Range Interactions	14
1. Particle Conserving Systems	15
a) Exact Results	15
b) Motion of Interfaces	16
2. Particle and Momentum Conserving Systems	16
a) Model Binary Fluid	16
b) Computer Simulations with Particle-to-Grid Methods	17
E. Microscopic-Shock Profiles: Exact Solution of a Non-Equilibrium System	18
IV. List of Publications supported by A.F.O.S.R. Grant: 1994 - August, 1997	20
V. Vita of Principal Investigator Publications of Principal Investigator	23

ABSTRACT

An improved understanding of equilibrium and non-equilibrium properties of plasmas is central to many areas of basic science as well as to the development and optimal utilization of plasmas in various technologies. This involves the study of the large variety of phenomena which take place when neutral, partially ionized atoms and electrons interact strongly with external fields and with each other in a plasma. It includes also the problem of creation and maintenance, with as efficient power use as possible, an extended plasma in the atmosphere such as is envisioned in the air plasma ramparts project.

We plan to continue our broad program of theoretical research in plasma physics based on the general principles of statistical mechanics and kinetic theory. These principles relate, via Gibbs ensembles and Boltzmann type equations, macroscopic phenomena of interest to the laws governing the microscopic constituents of matter. This includes dynamic phenomena such as the creation, maintenance and stability of nonequilibrium states, the absorption and emission of radiation, as well as fluctuations and phase transitions in equilibrium plasmas. We will be particularly interested in problems related to the physics and chemistry of air plasma ramparts.

Our work involves both rigorous mathematical analysis to find exact results whenever possible and suitable theoretical approximations for practical problems too difficult to analyze rigorously. Computer simulations also play an important role in our work, serving as a guide to theoretical developments and as a check on approximations.

I. Objective

An improved understanding of equilibrium and non-equilibrium properties of plasmas is central to many areas of basic science as well as to the development and optimal utilization of plasmas in various technologies. This involves the study of the large variety of phenomena which take place when neutral, partially ionized atoms and electrons interact strongly with external fields and with each other in a plasma. It includes also the problem of creation and maintenance, with as efficient power use as possible, an extended plasma in the atmosphere such as is envisioned in the air plasma ramparts project.

We plan to continue our broad program of theoretical research in plasma physics based on the general principles of statistical mechanics and kinetic theory. These principles relate, via Gibbs ensembles and Boltzmann type equations, macroscopic phenomena of interest to the laws governing the microscopic constituents of matter. This includes dynamic phenomena such as the creation, maintenance and stability of nonequilibrium states, the absorption and emission of radiation, as well as fluctuations and phase transitions in equilibrium plasmas. We will be particularly interested in problems related to the physics and chemistry of air plasma ramparts.

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II. Background and Approach

Statistical mechanics of equilibrium and non-equilibrium phenomena in general and of plasmas in particular aims at the coherent understanding of collective behavior of electrons, ions, and atoms, in as wide variety of physical situations as possible. To achieve this aim it couples the dynamics, specifying the basic rules governing the time evolution of the microscopic entities making up macroscopic matter, with statistical ideas taking into account the enormous number of atoms contributing to macroscopic behavior. The dynamical laws as well as the relevant statistics are governed by quantum mechanics although in many cases classical mechanics, which is generally easier to deal with, gives a very good approximation. This is however not always the case and many important problems in plasma physics involve quantum mechanics in essential ways. These include the ionization and recombination of atoms and molecules subject to external fields. Here we want to know how the transition between levels is affected by variations in the applied fields. This may also depend on how the level structure of isolated atoms or molecules is changed by the interactions with other particles in the system. These interactions can have large effects leading to the modification of some levels and possibly introducing new

kinds of metastable states. They are clearly relevant for many applications including the design of air plasma ramparts.

The actual behavior of the plasma, once it is established and maintained, can be studied for the most part by means of classical statistical mechanics. We are then led in many cases to the derivation and solution of appropriate Boltzmann type equations for the position and velocity distribution functions of particles undergoing both elastic and inelastic collisions. An important question which we have been studying is the nature and stability of solution of such kinetic equations in time dependent as well as stationary nonequilibrium situations. During the past few years we have succeeded in proving rigorously the existence of nonequilibrium phase transitions in weakly ionized plasmas subjected to external fields as well as to obtain rigorous bounds on the transport coefficients of such systems.

Due to the complexity of these problems it is often crucial to reduce the kinetic equations to more manageable hydrodynamic type equations involving only spatial coordinates and time. Examples include the (magneto) hydrodynamic equations used to describe the time evolution of spatially inhomogeneous (plasmas) fluids. We have achieved some success in obtaining such hydrodynamic equations rigorously from kinetic equations in appropriate scaling limits.

There are also situations in which it is more appropriate to bypass kinetic theory and use directly approaches based on general principles of statistical mechanics. Thus a plasma interacting with a laser field which is described, to a good approximation, by the Zakharov or the non-linear Schrödinger equations, has been studied by us successfully using the Gibbs ensemble approach. Similarly vortex motion in two dimensional fluids and magnetized plasmas can be studied via the equilibrium ensemble approach of Onsager. We are currently in the process investigating an apparently novel phase transition predicted by this theory and comparing it with experiments.

This work is part of our program for developing a general statistical mechanical theory for systems far from equilibrium. To achieve this goal and obtain a truly microscopic theory of phase transitions in nonequilibrium systems we have been studying also other representative examples of such phenomena. These are the microscopic structure of shocks and the kinetics of phase segregation. We have been able to obtain exact results for the former in some model systems. We have also derived, for the first time, exact macroscopic equations describing phase segregation in systems with long range interactions.

We hope that our work will answer questions such as the existence of suitable nonequilibrium free energy functionals, the validity of the fluctuation dissipation theorem and Onsager relations for the "pseudo" transport coefficients in a plasma in a more precise and useful way than is currently possible. The present approaches work either through analogies with equilibrium or through ad hoc prescriptions such as "minimum energy dissipation", "maximum entropy production", or "maximum likelihood" principles. These

"principles" seek in some ways to avoid the difficult task of solving the dynamic problem but it is not clear at present under what conditions they are valid and/or useful.

In summary we propose to continue and expand our statistical mechanical investigations on properties of interacting particle systems, with the aim of increasing understanding of the phenomena occurring in partially and fully ionized plasmas. Applications related to the creation and maintenance of air plasmas will be of particular concern. In what follows we give an outline of some projects we are pursuing and plan to carry out in the future.

III. Research

A. Energy Growth and Ionization in Driven Atomic Systems

We are interested in studying methods of dissociation and ionization of molecules present in, or easily added to the atmosphere. The objective is the creation and maintenance of a plasma in the air with minimum power expenditure. Our approach will use methods developed in the study of the phenomena of energy growth and other instabilities occurring in driven quantum systems. For the problem at hand these would correspond to going from a bound state to an ionized one. It has in fact been shown recently, using ideas developed in our previous work, that one could use this approach to obtain very efficient dissociation of certain molecules. (96% dissociation of a model HF molecule by a chirped infrared laser pulse of 2.3 ps duration and $10^3 \omega/cm^3$ intensity.)

A natural framework for the study of typical behavior of systems subjected to general time dependent fields, which includes periodic and almost periodic fields as special cases, is to write the Hamiltonian in the form

$$H(t) = H_0(x) + V(x; \xi_t) \quad (1)$$

Here x stands for the internal dynamical variables of the system and $\xi_t \in \Omega$ is a time dependent "external" classical variable, corresponding to the trajectory of a classical dynamical system on a domain Ω , having an invariant ergodic measure μ . One considers then typical or averaged behavior with respect to μ .

a) The Time-Periodic Case

The case of time-periodic external force, which in this language corresponds to Ω being a circle with $\xi_t = \xi + \omega t$, and $d\mu = d\xi/2\pi\omega$, has been studied most extensively both for classical and quantum systems. The stability problem can then be expressed in terms of the properties of the Floquet operator $U(t + T, t)$ which gives the evolution of the system over one period $T = 2\pi/\omega$. U is a unitary operator on the Hilbert space \mathcal{H} of the unperturbed system. The long time behavior of the system and its stability can be expressed in terms of the spectral properties of the Floquet operator. The energy remains bounded if the spectrum is pure point, and it grows unbounded if the spectrum is continuous. In our work we have obtained conditions under which these may occur.

b) General Time Dependence

A generalization of the Floquet theory connecting spectral and stability properties is not yet completely developed. Some progress has however been made. Let $U_\xi(t, s)$ be the propagator of the system described by the Hamiltonian (1) when ξ is a state of the classical dynamical system (Ω, ξ_t, μ) in which the evolution ξ_t is generated by an invertible flow

$$\xi_t = g(t)\xi$$

We then have

$$U_\xi(t + a, s + a) = U_{g(a)\xi}(t, s); \quad a \in \mathbb{R}$$

One considers then, in analogy with the periodic case, the enlarged space

$$\mathcal{K} = \mathcal{H} \otimes L_2(\Omega, d\mu)$$

and the one-parameter family of operators $W(t)$ acting on $\Psi(x, \xi) \in \mathcal{K}$

$$[W(t)\Psi](x, \xi) = U_\xi(0, -t)\Psi(x, g(-t)\xi).$$

$W(t)$ is a strongly continuous family of unitary operators and thus can be represented as

$$W(t) = e^{-iKt}$$

The self-adjoint generator K is the generalized quasi-energy operator. It acts as

$$[K\Psi](x, \xi) = -i \frac{d\Psi(x, g_t\xi)}{dt} \Big|_{t=0} + H(\xi)\Psi$$

We have been able to show that under appropriate conditions there is a correspondence between stability and the spectral properties of the generalized quasi-energy operator.

c) Dissociation by Chirped Laser Pulses

The use of chirped (or frequency-swept) laser pulses opens new possibilities of control in atomic and molecular physics. The essential tool is quasi-energy diagrams as a function of the laser amplitude and an effective frequency. The choice of the chirping evolution is guided by the analysis of the structure of the avoided crossing in the quasi-energy diagram. The method was successfully applied to the complete dissociation of a diatomic molecule by an ultrashort infrared chirped laser pulse. The total Hamiltonian acting on the Hilbert space $\mathcal{H} = L_2(\mathbb{R}, dx)$ is

$$\hat{H}(t) = H(\theta + \omega(t)t) \equiv H_0 - q\alpha(t) \sin(\theta + \omega(t)t),$$

The system is initially in its ground state φ_0 and the objective is to achieve complete transitions to an excited state φ_1 , which could be an ionized state by chirping. The first

essential point, phase (i), is to use a laser with a non-resonant frequency ω_i with respect to the ground state and the lower excited states, to avoid any crossing or avoided crossing in the quasi-energy diagram at zero field amplitude. This has the consequence that the initial population stays adiabatically completely concentrated in the single Floquet state Ψ_α , which is continuously connected to the ground state. In phase (ii), the frequency decreases from ω_i as described by a time dependent function $\omega(t)$. The Floquet Hamiltonian takes the form

$$K^{[\alpha, \omega_{eff}]}(\theta) = H(\theta) - i\hbar\omega_{eff}(t)\frac{\partial}{\partial\theta}. \quad (2)$$

with the effective frequency $\omega_{eff}(t) = \omega(t) + \dot{\omega}t$, which is the relevant one for the analysis of the quasi-energy diagram. As ω_{eff} decreases from ω_i to $\omega_{eff}(t_f)$, Ψ_α goes through an avoided crossing with Ψ_b . If the time dependence in $\omega_{eff}(t)$ is sufficiently slow, the Schrödinger evolution follows the instantaneous eigenvalue branch by continuity. This means that after the avoided crossing, the population that was originally in the state Ψ_α is in the instantaneous Floquet state Ψ_b . Phase (iii) is then used to reconnect the Floquet branches to the unperturbed states after the avoided crossing. Ψ_b is now linked by continuity to φ_1 and Ψ_α to φ_0 .

In order to achieve a complete transition from φ_0 to φ_1 , one needs a sufficiently slow pulse in order that all the population follows the Floquet states adiabatically during the increasing and decreasing phases of the pulse, and a sufficiently slow variation of the chirping $\omega_{eff}(t)$ near the avoided crossing. One thus designs a $\omega_{eff}(t)$ that is adapted to the location of the avoided crossings, and from it, one can easily deduce the chirping which needs to be implemented from Eq. (2).

B. Transport Processes in Plasmas

1. Bounds on the Mobility of Electrons in Weakly Ionized Plasmas

The behavior of the electron mobility in a gas composed of several species is a subject of continued experimental and theoretical investigations. Of particular interest is the fact that the *addition* of certain types of scatterers, i.e. neutral species, to the gas increases the electron mobility and therefore the electron current in an applied electric field. This effect is potentially of practical utility and can be used to obtain information about scattering cross sections and level structure of different species.

The fact that the mobility can actually increase with the addition of scatterers is at first surprising: it is contrary to the well known Matthiessen rule in metals which states that the total resistivity due to different types of scatterers is the sum of resistivities due to each of them. A closer inspection shows that Matthiessen's rule applies only to weak fields while the observations and analysis in gases are in the nonlinear high field regime.

This still leaves open the question of the validity of approximations commonly made in calculating the current of weakly ionized plasmas in strong fields. We therefore inves-

tigated rigorously the stationary solutions of the kinetic equation for the electron velocity distribution function in cases where the electron-neutral (e-n) collisions are purely elastic and their cross section is modeled by a simple power dependence on the electron speed. In particular we established two-sided bounds for the electron mean energy and drift in the presence of an external electric field. These bounds show that the results obtained for the current and energy of the electrons in the usual approximation, which neglects higher order terms in a Legendre polynomial expansion and gives the Druyvesteyn-like distribution for large fields, are qualitatively right and even provide good quantitative answers. In fact they are sufficiently precise to confirm an increase in the current for large (but not for small) fields upon addition of some gases, provided the mass of the added species is smaller than that of the dominant one, e.g. adding Helium to an Xenon gas, and the different cross sections satisfy certain conditions. We plan to extend our analysis to i) improve the accuracy of the bounds on electron mobility and energy; ii) include more realistic elastic cross sections and inelastic collisions; these are most important in practice for enhancement of the electron mobility; iii) take into account the recombination processes which play a significant role for dense/cold plasmas.

2. The Reflection of Electromagnetic Waves by a Conducting Surface Shielded with a Plasma Layer

The propagation of a monochromatic plane wave with frequency ω and electric vector amplitude $E(x)$ in the half-space $x \geq 0$ with a conducting surface at $x = 0$ was considered. The incident wave comes along the x -axis from $x = \infty$, where it has wavenumber k_0 , and travels through a plasma with a fixed density $n(x)$, $n(x) \rightarrow 0$ as $x \rightarrow \infty$. We are interested in the strength of the reflected wave for normal incidence.

Assuming the ionized layer to be much thicker than the Debye length, the problem was solved for two models:

1) The plasma density produces an exponentially decaying conductivity $\sigma(x)$ with the fixed real part of its dielectric constant the same as in vacuum. Such conductivity dependence corresponds to an exponential decrease of the plasma density $n(x)$ which could be a consequence of the plasma recombination obeying the linear law

$$D \frac{d^2 n}{dx^2} - \zeta n(x) = 0 \quad (1)$$

where $D = \text{const}$ is the diffusion coefficient and ζ presents the rate of recombination. The exponential model of plasma density allows an analytical solution, and it is therefore often used in studying the propagation of electromagnetic waves in the atmosphere. It is connected with the Chapman law in the ionosphere. A solvable version of this law, introduced by Epstein and treated in a more general context by Vidmar for the exploration of reflecting and transmitting properties of artificial plasma layers. While we do not

believe in the practical accessibility of exponential plasma profiles for the problem at hand, we study it for the better understanding of more practical plasma density distributions, including the final results of our calculation on the second model.

2) An approximately realistic description of a plasma layer generated near a metallic surface is considered. The plasma decay is assumed to be governed by the dissociative recombination of electrons with positive molecular ions. This is presumably the dominant process for cold weakly ionized plasmas. Since the incident wave is assumed weak enough for all processes to be linear, the plasma spatial profile may be determined first and then the reflection problem solved.

We plan to extend this work to more general cases. In particular, consider a plane wave incident on a medium whose dielectric and magnetic functions vary only in one direction, say z . The amplitudes of the electric field and magnetic field of the wave are then governed by a set of differential equations which can be written in a form

$$\frac{d^2\psi}{dz^2} + K^2(z)\psi = 0. \quad (2)$$

A popular numerical scheme for solving (2) is the partition of the inhomogeneous medium into thin layers ($j=1,2,3,\dots$) perpendicular to the z -axis, where the magnetic and dielectric functions are assumed constant and therefore $K_j = \text{const}$.

This method is not very effective numerically because it converges only linearly in terms of the layer thickness, or N^{-1} . When the plasma is strongly inhomogeneous one needs a large N for an accurate modeling of $K(z)$, and this is not only time consuming but also restricts the best possible accuracy due to accumulation of computation errors. The slow convergence of the scheme is caused by the sharp changes of $K(z)$ at the boundaries between adjacent layers.

Modeling of $K(z)$ by a continuous function can be expected to give a much better output. We therefore propose to approximate $K(z)$ in each layer j by $K_j(z) = a_j(b_j + z)^{-1}$. This will give

$$\psi_j = A_j(b_j + z)^{\gamma_j^+} + B_j(b_j + z)^{\gamma_j^-}, \quad (3)$$

with γ_j obtained from the equation $\gamma_j(\gamma_j - 1) + a_j^2 = 0$. The two free parameters, a_j, b_j allow us to have continuity of $K(z)$. Preliminary computer experiments show a tremendous advantage of this calculation method over the traditional one both in speed and accuracy.

We also note that in the generation phase of the plasma, the determination of the dielectric properties are much more complicated than in the stationary state of the plasma due to the strong inhomogeneities in this regime. A technique which may be useful here is **homogenization**, whose main purpose is to speed up significantly the computation of the transport properties by replacing a very complicated local problem with an effective nonlocal problem that gives the same overall results.

C. Phase Transitions and Instabilities

Introduction

The understanding of equilibrium phenomena, including their most interesting aspect, that of phase transitions, has enormously advanced in the past few decades. The elegant and precise theory of Gibbs measures provides a direct bridge between the microscopic and macroscopic descriptions of such systems. This includes a general conceptual framework as well as nontrivial explicit examples of the coexistence of multiple equilibrium phases for certain values of the macroscopic control parameters. In our earlier work supported by the AFOSR we have made considerable progress on the extension and development of equilibrium statistical mechanics of plasmas, although much remains to be done on phase transitions in charged systems—a problem we plan to investigate in the coming years.

Our understanding of nonequilibrium phenomena is far less advanced. In particular there is no general microscopic theory of nonequilibrium phase transitions. Our mathematical understanding of the great variety of nonequilibrium phase transitions observed in fluids, plasmas, lasers, etc., therefore depends mainly on the study of bifurcations and other singular phenomena occurring in the solutions of the nonlinear equations describing the *macroscopic* time evolution of such systems. One of the objectives of our work is therefore to develop a more microscopic theory of such phenomena. This program has met with a certain amount of success in recent years.

1. Phase Transitions in a Spatially Uniform Weakly Ionized Plasma

Instabilities are ubiquitous in strongly ionized plasmas. They dominate the behavior of such systems and their study forms the core of the subject. The origin of the instabilities lies in the nature of the plasma interactions: on the one hand they are long range and thus can produce strong cooperative effects and on the other hand they become 'weaker' locally at high energies (or temperatures) as manifested by the decrease of the Coulomb cross section with energy rise. The situation is different in weakly ionized cold plasmas, systems which have attracted much attention recently. In such systems, collective phenomena play a smaller role and instabilities are less common. Nevertheless there are cooperative phenomena in these systems too, which can lead to dramatic abrupt changes in the state of the plasma, e.g. nonequilibrium phase transitions, when such systems are driven by external fields,

In recent years we succeeded in obtaining a rigorous mathematical proof of a phase transition for such a weakly ionized plasma. Our set up is as follows: We consider a weakly ionized gas in the presence of an externally imposed constant electric field E . The density of the gas, the degree of ionization and the strength of the field are assumed to be such that: (i) the interactions between the electrons can be described by some nonlinear, Boltzmann type collision operator, and (ii) collisions between the electrons and the heavy components of the plasma, ions and neutrals, are adequately described by assuming the

latter ones to have a spatially homogeneous time independent Maxwellian distribution with an a priori given temperature. Under these conditions the time evolution of the spatially homogeneous velocity distribution function $f(v, t)$ will satisfy a Boltzmann type equation

$$\frac{\partial f(v, t)}{\partial t} = -E \cdot \nabla f + Lf + \epsilon^{-1} Q(f), \quad (1)$$

where ∇ is the gradient with respect to v , E is a constant force field and Q is a nonlinear collision term.

We proved that there exist multiple stationary distributions $f(v)$ which are solutions of the non-linear kinetic equation (1). These occur in the vicinity of any one of the stable fixed points on the hysteresis loop obtained from the solution of a pair of nonlinear equations for the hydrodynamical variables; current and temperature. We showed furthermore when the system is started near such a stable hydrodynamic state it will remain there forever. If, on the contrary, it is started near the unstable fixed point, it will leave the neighborhood after some finite time.

To put the above results in context we note that while there has been much progress recently in deriving hydrodynamic equations from simple microscopic and even realistic mesoscopic model evolutions the passage to the macroscopic scale is well understood *only over time intervals in which the solutions of the macroscopic equations stay smooth*. The reason for this is that control of the error terms in the estimates depends on *a-priori* smoothness estimates for solutions of the macroscopic equations. Thus, they shed no light on the actual behavior of the mesoscopic description when the solutions of the hydrodynamical equations develop singular behavior.

To overcome this problem it is clearly desirable to develop methods in which one does not use any *a-priori* smoothness estimates for solutions of the macroscopic equations, but instead uses scale independent estimates on the kinetic equation. This is what we did for the model of a plasma in an external field described by (1) where we proved that kinetic description closely tracks the macroscopic one even when the driving is sufficiently strong for the latter to undergo phase transitions. More precisely, we showed that the velocity distribution function is close to a Maxwellian parametrized by a temperature T and mean velocity u which satisfy certain non-linear equations, which are the macroscopic equations for this system. Moreover, it does so globally in time, even when the stationary solutions of these macroscopic equations are nonunique.

To show the stability of these multiple stationary solutions we need results that guarantee that a solution of the kinetic equations will stay near a solution of the macroscopic equations globally in time. This seems to be difficult to accomplish by standard expansion methods, at least in the range of driving field strengths where the macroscopic equations have the most interesting behavior. Instead of expansion methods, we used entropy production to show that the solution of the kinetic equations must stay close to *some*

Maxwellian, globally in time. Then, we showed that the moments of this Maxwellian must nearly satisfy the macroscopic equations. In this way we got our results.

In the coming period we plan to extend these results to more realistic situations. Partial progress in this direction for a nonuniform plasma are described in the next section.

2. Phase Transition in a Cylindrical Plasma

We have partially extended our investigations of phase transitions in weakly ionized plasmas to more realistic experimental conditions than the spatially homogeneous weakly ionized plasma considered earlier.

We consider an experimental arrangement consisting of a weakly ionized gas in a tube of radius R subjected to a constant external axial electric field E . The plasma is assumed for simplicity to be produced through uniform ionization inside the tube, by some external source, at a constant rate α . It is balanced by two kinds of recombination processes: a bulk one and a surface process on the tube wall. The main bulk recombination for the regime we are interested in, are three body processes involving two electrons plus an ion, and dissociative recombinations in which a metastable atom-ion complex recombines with an electron. The rates depend on the temperatures and densities of the electrons, ions and neutrals in a rather complicated way. For the sake of simplicity we lump the two processes together and assume an effective rate of bulk recombination proportional to $T^{-3/2}$, where T is the electron temperature. We ignore the dependence of this rate on the neutral and ion temperature and on the pressure that we keep more or less constant. The recombination at the wall is also treated phenomenologically. In particular we assume that the energy is absorbed by the wall that is kept at a fixed temperature.

We have in mind here a situation in which the great majority of neutral atoms are some kind of noble gas to which may, or may not, be added a small amount of a more easily ionized second species, though we realize that in the latter case the analysis would be more complicated. This will be reflected mainly in the rates of ionization α and recombination γ since we shall always consider a regime in which the density of electrons $n(r, t)$ is much lower than that of the neutrals, N , but big enough, due to the great disparity between the electron mass, m , and the ion-neutral mass, M , for binary electron-electron collisions to dominate the energy exchanges in electron-ion and electron-neutral (e-i and e-n) collisions. This requires that

$$\frac{\sigma m}{2\pi M e^4} (kT)^2 \ll \frac{n}{N} \ll 1. \quad (2a)$$

Here k is the Boltzmann constant, and σ is the total electron-neutral particle collision cross section, which is taken to be a constant in our work. Putting in appropriate values for the parameters on the left side of (2a) gives

$$1 \gg n/N \gg 8 \cdot 10^{-7}, 4 \cdot 10^{-8}, 1.5 \cdot 10^{-8} \quad (2b)$$

for He, Ne, Ar plasmas respectively, when kT is approximately 1 eV and it decreases as T^2 for colder electrons. The upper bound relates to the fact that we ignore any collective self-induced electrostatic or magnetic interactions.

The ions in our model are assumed to have a uniform temperature, T_i , the same as the neutrals, while their density is $n(r, t)$, i.e., the plasma is treated as locally quasi-neutral. We assume axial symmetry and longitudinal homogeneity so the spatial dependence is only in the radial variable $r \leq R$. The different mobilities of ions and electrons are compensated by an internally generated radial ambipolar electric field $F(r, t)$. We are thinking of a quiescent, long positive column which fills the tube.

The reason for considering external rather than field-induced ionization is that the transition in the electron distribution between regimes of weak and strong coupling to the ions as we vary the external field E found in our previous work requires a low electron temperature and relatively weak electric field, which seems hard to achieve when the ionization is produced by the field.

The basic idea is again to consider situations in which the collisions between electrons are strong enough to force their velocity distribution $f(r, v, t)$ to stay close to a Maxwellian with temperature T and drift velocity w . The values of T and w , which are simply related to the first two velocity moments of f , are then determined by self consistent "hydrodynamic" equations, i.e. we evaluate the integrals entering the time evolution of T and w with the help of replacing f by this Maxwellian. For the spatially homogeneous case this yields ordinary differential equations in time for T and w that can be reduced to a couple of transcendental equations for stationary values $T(E)$ and $w(E)$ yielding, in some cases, S-shaped curves as functions of $E = |E|$. In the inhomogeneous situation we obtain nonlinear partial differential equations for $n(r, t)$, $T(r, t)$, $w(r, t)$ and the radial electric field (or the plasma ambipolar field). Their stationary solutions again exhibit regions where the system is unstable. The physical situations where this transition might be observed is a much more restrictive domain than that given by (2), it requires essentially $n/N \sim 10^{-4}$ while $N \sim 10^{15} \text{ cm}^{-3}$ for light noble gases when T_i is close to room temperature. At the transition the electron temperature jumps within a range of several T_i , staying significantly lower than the usual temperatures in self-sustaining gas discharges. This determines the experimental setup required to see this instability.

3. Transitions between Shear and Vortex Flows in Statistical Hydrodynamics

The motion of N point vortices embedded in a two-dimensional incompressible inviscid fluid is governed by the Hamiltonian dynamics $c_i \dot{\mathbf{r}}_i = J \cdot \nabla_i H^{(N)}$, where c_i is the circulation and $\mathbf{r}_i = (x_i, y_i) \in \Lambda \subset \mathbb{R}^2$ the position of the i -th vortex, J is the symplectic matrix, and $H^{(N)}$ the point vortex Hamiltonian, given by

$$H^{(N)}(\mathbf{r}_1, \dots, \mathbf{r}_N) = \sum_{1 \leq i < j \leq N} c_i c_j G(\mathbf{r}_i, \mathbf{r}_j) + \sum_{1 \leq i \leq N} c_i^2 F(\mathbf{r}_i) \quad (3)$$

$$F(\mathbf{r}) = \lim_{\tilde{\mathbf{r}} \rightarrow \mathbf{r}} \frac{1}{2} \left[G(\tilde{\mathbf{r}}, \mathbf{r}) + \frac{1}{2\pi} \ln |\tilde{\mathbf{r}} - \mathbf{r}| \right] \quad (4)$$

In (3), G is a Green's function for $-\Delta$ on Λ . Its precise form depends on the geometry and topology of Λ and, if Λ has a boundary $\partial\Lambda$, on the boundary conditions. In a pioneering paper, Onsager pointed out the potential significance of the statistical equilibrium distribution $\delta(H^{(N)} - E)$ of (3) for two-dimensional fluid flows. Onsager's theory yields a distinguished class of stationary incompressible Euler flows in the limit $N \rightarrow \infty$ in a fixed domain Λ , with energy scaled so that $\epsilon = E/N^2$ is fixed. This limit was constructed recently by us using a Gaussian ensemble. The flows satisfy a set of nonlinear equations derived previously via a mean-field approximation to $\delta(H^{(N)} - E)$. This theory has been remarkably successful in reproducing in a quantitative way the almost stationary vorticity structures at intermediate times of a high Reynolds number Navier-Stokes simulation on a doubly periodic lattice. Here, "intermediate times" means time that are long compared to an eddy turnover time and short compared to the overall viscous decay time. The success of mean-field theory in this particular situation suggests it be evaluated in a systematic way, looking for new interesting predictions like phase transitions, and comparing it with further simulation results.

In work in progress we carry out such an analysis for various realizations of the mean-field model equations in rectangular domains which are frequently employed in numerical simulations. A systematic evaluation has so far been carried out for one-species systems in all space, and in circular domains. In circular domains a phase transition has been found. It has been qualitatively associated with the observable phenomenon of the diocotron mode in the electron guiding center plasma, whose dynamics approximates vortex flows.

We have also studied neutral systems on doubly periodic lattices. We find several phase transitions between different vortex flows and shear flows, depending on the aspect ratio of the lattice. We also treat various systems on periodic strips. Here too we find a phase transition between shear and vortex flows. These results qualitatively reproduce various numerical simulations.

4. Instabilities in Plasmas Interacting with Lasers

The difficulties encountered in constructing statistical mechanical theories of nonequilibrium systems are associated with their potentiality for various kinds of instabilities. This is indeed the case for plasmas irradiated with laser light. Here the collective modes represent Langmuir waves and the instability is the soliton or caviton collapse which gives rise to plasma turbulence. The physics of the problem—including the reasons for expecting an equilibrium treatment of the collective modes to be of any relevance, even though the system is clearly not in thermodynamic equilibrium—are described by the Zakharov model, which contains the ion acoustic waves in addition to Langmuir waves.

In earlier work we investigated the statistical mechanics of a simplified version of this system, i.e. complex field whose dynamics are governed by the non-linear Schrödinger equation. The Hamiltonian is unbounded below and the system will, under certain conditions, develop (self-focusing) singularities in a finite time. We showed that, under certain conditions, the Gibbs measure is absolutely continuous with respect to Wiener measure and normalizable if and only if classical solutions exist for all time — no collapse of the solitons. We have also investigated a mean field type Gaussian ensemble which furnishes a good approximation to this measure over a wide range of parameters. These works have had quite a wide impact and various extensions of them have recently appeared in the literature. We plan to continue this work in several directions, rigorous and computational.

Computations have played an essential role in this work, both in determining the properties of the true ensemble via Monte Carlo simulations and in solving the fixed point problem arising in the Gaussian approximation. Further work will involve additional computation. One project is to simulate the dynamics of the nonlinear Schrödinger equation itself, and compare the statistics collected from a typical trajectory with the statistics in the ensemble; we hope that this will lead to deeper understanding of the significance of the temperature parameter in the Gibbs measure. We are also interested in constructing the measure in higher dimensions, where extensive Monte Carlo studies will undoubtedly be necessary.

D. Phase Segregation Dynamics in Particle Systems with Long Range Interactions

Introduction

The process of phase segregation through which a system evolves towards equilibrium following a quench from a high temperature homogeneous phase into a two phase region of its phase diagram has been of continuing interest during the last decades, but many problems still remain to be solved. This is particularly so for fluids, when particle, momentum, and energy densities are conserved locally; these are currently the focus of both numerical studies and experiments.

1. Particle Conserving Systems

a) Exact Results

During the period of the last grant we rigorously derived a macroscopic equation describing the time evolution of the empirical average process, i.e. the local density, for a model of interacting particles with one conservation law undergoing phase segregation.

The particle models are dynamic versions of lattice gases with long range Kac potentials. By a long range Kac potential, we mean that the interaction energy between two particles, say between a particle at x and one at y (x and y are both in d -dimensional simple cubic lattice \mathbb{Z}^d), is given by $\gamma^d J(\gamma(x - y))$, where J is a smooth compactly supported function ($J(r) = J(-r)$) and γ is a positive parameter which is sent to zero. The equilibrium states for these models have been investigated thoroughly and have provided great mathematical insight into the static aspects of phase transition phenomena. The dynamical version of these models, in which each particle jumps at random times from a site of the lattice \mathbb{Z}^d to one of its unoccupied nearest neighbor sites is sometimes called *local mean field Kawasaki dynamics*. The jump times are chosen according to a probability distribution which depends on the particle configuration and is reversible with respect to the equilibrium Gibbs measure. To find a hydrodynamic scaling limit, we scale also the lattice spacing with γ and the time with γ^{-2} (this is the so called *diffusive limit*). We then derive a (deterministic) evolution law for the macroscopic density ρ .

We believe, but have not yet proven, that our results can be extended to more general cases including even plasmas where the Coulomb potential is formally of the Kac type. The resulting evolution is given in terms of a second order integrodifferential equation:

$$\partial_t \rho(r, t) = \nabla \cdot \left[\sigma(\rho) \nabla \left(\frac{\delta \mathcal{F}}{\delta \rho} \right) \right] \quad (5)$$

ρ is the density, σ (a function of ρ) is the mobility and

$$\mathcal{F}(\rho) = \int_{T^d} f_c(\rho(r)) dr + \frac{1}{4} \int \int_{T^d \times T^d} J(r - r') [\rho(r) - \rho(r')]^2 dr dr' \quad (6)$$

in which f_c is either convex or it has a symmetric double well structure, with minima at ρ^- and ρ^+ . The latter will be the relevant case for us: we will call the densities ρ^- and ρ^+ the *phases* of the system. The dependence on the temperature (of σ and f_c) is suppressed. In probabilistic terms, (5) is a law of large numbers for the empirical averages over the particle system. Equation (6) is in a particularly enlightening form: it is the gradient flux associated with the classical local mean field free energy functional, with a density dependent mobility σ . The form of equation allows us to connect the concepts of critical temperature, phases, stable, unstable and metastable states of the model, with the properties of the solutions of the evolution equation. The next step is to understand the

evolution of the boundaries (interfaces) between regions in which the density is close to ρ^\pm .

b) Motion of Interfaces

Formal matched asymptotic expansions, in the so called *sharp interface limit*, of the solution of macroscopic evolution equations have been successfully employed to understand the interface motion in several models. By *sharp interface* we mean the limit in which the phase domains are very large with respect to the size of the interfacial region: if we denote by L the *typical* size of the domains, we will look for results in the limit $L \rightarrow \infty$. The time will have to be properly scaled as well, typically as some integer power of L , according to the type of initial condition.

The general picture that we obtain for the interface motion is the following: choose an initial condition which takes only metastable or stable values over large domains (of typical diameter $O(L)$), while the interfacial regions are layers of thickness $O(1)$ and let it evolve according to (5). There is, first, the equilibration of the interface which happens on a fast time scale ($t \ll L^2$). Then, on the time scale $t \propto L^2$ the evolution of the density in the bulks (that is the interior of the domains) is given by a nondegenerate nonlinear diffusion equation with Dirichlet boundary conditions on a free boundary, the interface (*Stefan problem*). Once the density in the bulks is relaxed to the density of the phases, the motion of the interface on this time scale stops. A slower evolution can then be seen on the time scale $t \propto L^3$ and the motion of the interfaces is given by the Mullins–Sekerka model; a quasistatic free boundary problem in which the mean curvature of the interface plays a fundamental role.

2. Particle and Momentum Conserving Systems

a) Model Binary Fluid

We carried out investigations of spinodal decomposition in a three-dimensional mixture of two kinds of particles that we label 1 and 2 using a novel microscopic dynamics and computational scheme. The particles interact with each other through short range interactions modeled here by hard spheres having the same mass m and diameter d . Particles of different kinds interact also through a long range repulsive Kac potential, $V(r) = \gamma^3 U(\gamma r)$. The equilibrium properties of such a system are well understood, there is even a rigorous proof of a phase transition at low temperatures to an immiscible state, which in the limit $\gamma \rightarrow 0$, is described by mean field theory. When the density n is low enough, $nd^3 \ll 1$, and the potential sufficiently long ranged, $n\gamma^{-3} \gg 1$, the free energy of the system is well approximated by $F = k_B T \int [n_1(\vec{r}) \ln n_1(\vec{r}) + n_2(\vec{r}) \ln n_2(\vec{r})] d\vec{r} + \int V(|\vec{r}_1 - \vec{r}_2|) n_1(\vec{r}_1) n_2(\vec{r}_2) d\vec{r}_1 d\vec{r}_2$. The $\gamma \rightarrow 0$ critical temperature, which should be an upper bound for T_c^γ at $\gamma > 0$, is given by $\frac{k_B T_c^0 = 1}{2n \int U(r) d\vec{r}}$. In this regime the dynamical evolution of the

system should be well described by two coupled Boltzmann - Vlasov equations:

$$\frac{\partial f_i}{\partial t} + \vec{v} \cdot \frac{\partial f_i}{\partial \vec{r}} + \frac{\vec{F}_i}{m} \cdot \frac{\partial f_i}{\partial \vec{v}} = J[f_i, f_1 + f_2], \quad i = 1, 2 \quad (7)$$

where $f_i(\vec{r}, \vec{v}, t)$ are the one-particle distribution functions, $\vec{F}_i(\vec{r}, t) = -\nabla \int V(|\vec{r} - \vec{r}'|) n_j(\vec{r}') d\vec{r}'$, $n_j(\vec{r}') = \int f_j(\vec{r}', \vec{v}, t) d\vec{v}$ with $i, j = 1, 2, i \neq j$, and $J[f, g]$ is the Boltzmann collision operator for hard core interactions. Kinetic equations of this type have been proposed, and if the system is quenched inside the coexistence region they will describe gas-gas segregation into two phases, one rich in particles of type 1 and the other rich in particles of type 2. (Examples of gas mixtures that have a miscibility gap are helium-hydrogen, helium-nitrogen, neon-xenon etc..) We believe that the model contains the essential features of phase separation in general binary fluid mixtures.

b) Computer Simulations with Particle-to-Grid Methods

To simulate our system we modeled the Boltzmann collisional part using a stochastic algorithm due to Bird, known as Direct Simulation Monte Carlo (DSMC), while for the Vlasov part we used the particle-to-grid-weighting method, well known in plasma physics. In the DSMC method the physical space is divided into cells containing typically tens of particles. The main ingredients of this procedure are the alternation of free flow over a time interval Δt and representative collisions among pairs of particles sharing the same cell. In the particle-to-grid-weighting algorithm the particle densities are computed on a spatial grid through some weighting depending on the particle position, then the Vlasov forces are calculated on the same grid. Finally, the forces at the position of each particle are interpolated from the forces on the grid. The coupling of these methods, which have been extensively used individually, made possible our simulations of phase segregation with 1.4×10^6 particles, with only modest computational resources: a typical run took about 32 CPU hours on a 233 MHz Alpha Station. It appears that this method can be extended to the study of the effects of phase segregation on inhomogeneous hydrodynamical flows of practical importance.

Since one of our main interests was the late time hydrodynamical regime, a delicate balance had to be struck between the size of the system, the range of the potential, the temperature and the particle density, making sure that each of the methods is used within its range of validity and that their combination remains computer manageable. On the one hand the potential must be reasonably long ranged so that the Vlasov description is physically appropriate and numerically sound, and on the other hand it must have a range much smaller than the size of the system. This restriction made necessary the use of two spatial grids: a somewhat coarse one for the collisions and a finer grid for the long range potential. It also imposed the use of quadratic spline interpolation for the calculation of grid quantities and a ten-point difference scheme for the calculation of the forces.

Our results were obtained using a system with 1,382,400 particles in a cube with periodic boundary conditions. We also studied smaller systems to identify unavoidable finite-size effects. The interaction potential used was Gaussian, $U(x) = \alpha \pi^{-\frac{3}{2}} e^{-x^2}$, $\alpha > 0$, but there is no reason to believe that different repulsive potentials would qualitatively change the results. All quenches were performed at a total particle density $nd^3 \simeq 0.01$ and an initial temperature T_0 , $T_0/T_c^0 = 0.5$. The initial conditions for each run were random positions for all particles and velocities distributed according to a Maxwellian of constant temperature. (In the DSMC evolution, as in the Boltzmann-Vlasov equations, the hard cores only enter in determining the collision cross sections.) The total energy of the system was very well conserved by the dynamics. This meant that the kinetic energy and hence the temperature increased as the system segregated, but at late times it changed very slowly on the time scale of our simulations. The effective number of particles in the range of the potential was about 100-500. The results of our simulations are presented in Figures 1-4.

E. Microscopic – Shock Profiles : Exact Solution of a Non – Equilibrium System

There is much interest, physical and mathematical, in the behavior of models systems of particles described macroscopically by a continuous density field satisfying equations of hydrodynamic type which produce shocks. In such cases it is clear that the hydrodynamic equations do not tell the full story; in fact, because of the discontinuities in the density and consequent infinities in the derivatives which enter the equations, shocks correspond to non-unique weak solutions of these equations, and, to find the physical solution, the equations have to be supplemented by additional conditions or be treated as the limit of equations with non-zero viscosity. The microscopic level has of course no room for such extra conditions and its study is therefore essential for a complete understanding of the behavior of shocks.

Unfortunately, even molecular-dynamics simulations of shocks in real particle systems can only be carried out very partially with the currently available supercomputers, so model systems such as the one-dimensional asymmetric simple exclusion process are important. In this model, particles on the lattice jump independently at random times with rate 1 to adjacent sites, choosing the site to their right with probability p , and to their left with probability $1 - p$, provided the target site is unoccupied. The density profile of this system on macroscopic spatial and temporal scales x and t is described for $p \neq 1/2$ in the appropriate hydrodynamic scaling limit by the inviscid Burgers' equation

$$\frac{\partial u(x,t)}{\partial t} + (2p - 1) \frac{\partial}{\partial x} [u(1 - u)] = 0. \quad (8)$$

This means that there exists a limiting scaling for which the actual random microscopic density exactly tracks the solution of the Burgers' equation.

This equation can produce shocks; for example, there is a solution of (8) such that $u(x, t) = u_+$ for $x > x_0(t)$ and $u(x, t) = u_-$ for $x < x_0(t)$, where $u_+ > u_-$ (when $p > 1/2$) and the shock position $x_0(t)$ moves with the constant velocity $(2p - 1)(1 - u_+ - u_-)$. We now ask about the corresponding microscopic behavior: can one see an abrupt change at that scale or is the jump in densities spread out over very large microscopic distances?

To analyze the shock microscopically one must first locate it—that is, define precisely its position—on the microscopic level. This may be done by introducing a special *second-class particle* into the system, which evolves by a modified dynamical rule: it behaves like a regular (first-class) particle when jumping to an empty site but must give way to any regular particle that tries to jump on it (by exchanging places with the latter). For $p > 1/2$ this dynamics makes the velocity of the second-class particle decrease with density and then gives it a drift towards regions of positive density gradient. This keeps the second-class particle near the shock and its position may then conveniently be taken as the definition of the (microscopic) shock location. With this definition it has been established that shocks are sharp even on the microscopic level; specifically, that the microscopic (ensemble-averaged) particle density at site j , as viewed from the second-class particle, has a time-invariant distribution which approaches the densities $\rho_{\pm} = u_{\pm}$ at $\pm\infty$.

In our recent work we have obtained the exact microscopic structure of such shocks. We obtain our results by first finding the exact stationary state of the system as seen from the second class particle. We find that the correlations decay exponentially when $\rho_+ > \rho_-$. In practice, this means that one can see the discontinuity on the scale of a few intermolecular distances, something consistent with computer simulations on real particle systems and with experiments. We also find that the “width” of the shock diverges as $\rho_+ \rightarrow \rho_-$.

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SUPPORTED BY AFOSR GRANT

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- [2] Nonunique Stationary States in Driven Collisional Systems with Application to Plasmas, (with E. Carlen, R. Esposito, R. Marra and A.V. Rokhlenko), *Phys. Rev. E*, 52, 40-43, 1995.
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- [39] Statistical Mechanics of Weakly Dissipative Current-Carrying Plasma, M. Kiessling, *Habilitation Thesis*, Ruhr University Bochum, 1995.

CURRICULUM VITA

LEBOWITZ, Joel L.

George William Hill Professor of Mathematics and Physics,
Director, Center for Mathematical Sciences Research,
Rutgers, The State University of New Jersey, New Brunswick

PII Redacted

EDUCATION:

B.S., Brooklyn College, 1952
M.S., Syracuse University, 1955
Ph.D., Syracuse University, 1956
NSF Postdoctoral Fellow, Yale University, 1956-57

POSITIONS:

Stevens Institute of Technology, Assistant Professor of Physics, 1957-59
Belfer Graduate School of Science, Yeshiva University,
Assistant Professor of Physics, 1959-60;
Associate Professor, 1960-65; Professor, 1965-77;
Chair, Department of Physics, 1968-76
Rutgers University, Professor of Mathematics and Physics,
Director, Center for Mathematical Sciences Research, 1977-

VISITING POSITIONS:

Cornell Graduate School of Medical Sciences, Visiting Scientist, 1965-73
American Telephone and Telegraph, Consultant, 1968-77
Institute des Hautes Etudes Scientifiques, Bures-sur Yvette, Guggenheim Fellow, 1976-77;
Visiting Scientist, Fall 1980, Fall 1988, Spring 1993, Spring 1997
Los Alamos National Laboratories, Consultant, 1978-
Institute for Advanced Study, Visiting Scientist, Spring 1981
Courant Institute, Visiting Scientist, (short periods), 1965-

EDITORIAL POSITIONS:

Editor-in-Chief, Journal of Statistical Physics, 1975-
Editor/Co-Editor, Annals of The New York Academy of Sciences, Collective Phenomena,
1980-1992

Co-Editor:

(with C. Domb) Phase Transitions and Critical Phenomena, Academic Press 1980-
(with E. Montroll) Studies in Statistical Mechanics, North Holland, 1973-1983; Editor 1984-

Editorial Board:

Communications in Mathematical Physics, 1973-
Journal of Mathematical Physics, 1966-69; 1993-
KINAM, 1978-1986
Physica D, 1978-1982, Advisory Board, 1983
Transport Theory and Statistical Physics, 1982-Physical Review A, 1984-87
Reports on Mathematical Physics, 1985-88
Progress in Mathematical Physics, 1989-
Letters in Mathematical Physics, 1993-

AFFILIATIONS AND HONORS:

National Academy of Sciences, Member 1980-
 New York Academy of Sciences, Board of Governors 1971-82;
 Vice-President 1974-76; President 1979
 Chairman, Publication - Conference Liaison Committee 1980-85;
 Chairman of Human Rights Committee 1980-93
 International Union of Pure and Applied Physics, Commission on Thermodynamics
 and Statistical Mechanics, Member 1979-81; Secretary 1982-84, President 1985-87
 Committee of Concerned Scientists, Co-Chairman, 1982-
 Distinguished Alumni Award, Brooklyn College of the City University of New York, 1969
 Guggenheim Fellowship, 1976-77
 Doctor Honoris Causa, Ecole Polytechnique Federale, Lausanne, 1977
 Fellow, American Physical Society, New York Academy of Sciences, American Association
 for the Advancement of Science: Member Phi Beta Kappa
 The A. Cressy Morrison Award in Natural Sciences for 1986, The New York Academy
 of Sciences
 Boltzmann Medal for 1992, IUPAP Commission on Thermodynamics and Statistical Physics
 College of Arts and Sciences Distinguished Alumni Award, Syracuse University, 1993
 Max Planck Research Award, Alexander von Humboldt Foundation, 1993
 Board of Trustees Award for Excellence in Research, Rutgers University, 1993
 Delmar S. Fahrney Medal, The Franklin Institute, 1995
 The 1996 Heinz R. Pagels Human Rights of Scientists Award of New York Academy of Sciences,
 1996
 The Rutgers College Class of 1962 Public Service Award, 1997

MEMBER OF:

Institute des Hautes Etudes Scientifiques, Bures-sur-Yvette, France, Scientific Committee
 for Scientific Matters, 1979-82
 Institute for Theoretical Physics, Santa Barbara, California, Advisory Board 1984-87
 International Association of Mathematical Physics, Executive Committee, 1982-87
 American Institute of Physics, Ad Hoc Committee for the Journal of Mathematical Physics,
 1970, 1978, 1984; Committee on Selection of Dannie Heineman Prize, Vice Chair, 1989,
 Chair, 1990
 American Physical Society, Committee on the International Freedom of Scientists, 1984-85
 Committee on Physical Review A, 1991, Chair
 National Academy of Sciences, Research Briefing Panel on Mathematics, Office of
 Science and Technology Policy, 1982
 International Sakharov Hearings, 1979
 Lars Onsager Memorial Prize Committee, 1994-
 Miller Research Fellows Advisory Board, University of California, Berkeley, 1984-86
 Open Society Fund, Fellowship Selection Committee, New York, 1982-
 J. van Neumann Computing Center, Board of Governors, 1987-1990
 American Mathematical Society, Committee on Human Rights of Mathematicians, 1988-91,
 Committee on Science Policy, 1990-92
 International League for Human Rights, Member of the Board, 1987-1988
 Association of Engineers and Scientists for New Americans, Joint Advisory Committee/Reference
 Team of the Refugee Scientist Program

Evaluation Committee, Physics, Harvard College, 1990-1993
 Evaluation Committee, Math and Phys, Clarkson University, 1986-
 Scientific Reviewing Committee at the Weizmann Institute of Science, 1995
 Self-Study Committee, Department of Physics and Astronomy, Lehman College of the
 City University of New York, 1995

CONFERENCE ORGANIZATIONS:

Advisory Organizing Committee:
 International Conference on Mathematical Physics, Berlin, 1981; Colorado, 1983;
 Marseille, 1986; Swansea, 1988; Paris, 1994
 International Conference on Thermodynamics and Statistical Mechanics, Edinburgh, 1983;
 Boston, 1986; Rio de Janeiro, 1989; Berlin, 1992; China, 1995, Paris 1998
 Colloquium and Workshop on Random Fields: Rigorous Results in Statistical Physics,
 Esztergon, 1979; Koszeg, 1984
 Conference on Mathematical Problems from the Physics of Fluids, Universita Degli Studi di
 Roma, 1985
 Conference on Statistical Mechanics and Field Theory: Mathematical Aspects, Groningen,
 1985
 Symposium on Statistical Mechanics of Phase Transitions: Mathematical and Physical
 Aspects, Trebon, Czechoslovakia, 1986
 International Advisory Committee and Conference Organizer for the Landau Memorial
 Conference on the Frontiers of Physics, 1988
 Models for Non-Classical Reaction Rates, National Institutes of Health, Bethesda, MD, 1991
 International A.D. Sakharov Conference on Physics, Moscow, USSR, 1991, 1996
 Lattice Gas Automata Workshop, Nice, France, 1991
 Workshop on Phase Transitions: Physics, Mathematics, Biology, Prague, Czechoslovakia, 1992
 International Conference on Three Levels, Leuven, Belgium, 1993
 Statistical Mechanics as a Branch of the Probability Theory,
 in memory of Roland L. Dobrushin, Vienna,, September 1996
 Mathematical Problems in Statistical Mechanics, Marseille, July 1997

INVITED CONFERENCE LECTURES (Partial List)

1991:

Microscopic Simulations of Complex Hydrodynamic Phenomena, Alghero
 International Symposium on Phase Transitions, Tel Aviv
 Advanced Research Workshop Lattice Gas Automata, Nice
 Physical Origin of Time Asymmetry, Mazagon, Spain
 Models of Non-Classical Reaction Rates, NIH

1992:

Symposium on Quantum Nonintegrability, Drexel (May)
 Workshop on the Theory of Phase Transitions, Prague (June)
 The State of Matter, Copenhagen (August)
 IUPAP International Conference on Thermodynamics and Statistical Mechanics,
 Berlin (August)
 Kinetics of Phase Transitions, Edinburgh (August)

1993:

The Statistical Mechanics of Fluids, Oxford (March)
 Dynamics of Complex Systems, Rome, May 17, 1993
 Advances in Dynamical Systems and Quantum Physics, Capri (May)
 Coupled Transport Processes and Phase Transitions, Trondheim (June)

1994:

Boltzmann Symposium, Austria (February)
 Boltzmann Symposium, Rome (May)
 Cellular Automata, Aggregation and Growth, U.K. (May/June)
 XIII Sitges Conference, Barcelona (June)
 11th Congress of Mathematical Physics, Paris (July) (Session Organizer)
 Symposium on Classical & Quantum Billiards, Switzerland (July)
 4th Drexel Symposium on Quantum Nonintegrability, Philadelphia (September)
 CAM (The Canadian, American and Mexican Physical Society),
 Cancun, Mexico (September)

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